

More on the Weeks Method for the Numerical Inversion of the Laplace Transform

G. Giunta, G. Laccetti, and M.R. Rizzardi

Dipartimento di Matematica e Applicazioni, Università di Napoli, Via Mezzocannone 16, I-80134 Napoli, Italy

Summary. Most of the numerical methods for the inversion of the Laplace Transform require the values of several incidental parameters. Generally, these parameters are related to the properties of the algorithm and to the analytical properties of the Laplace Transform function F(s).

One of the most promising inversion methods, the Weeks methods, computes the inverse function f(t) as a series expansion of Laguerre functions involving two parameters, usually denoted by σ and b. In this paper we characterize the optimal choice b_{opt} of b, which maximizes the rate of convergence of the series, in terms of the location of the singularities of F(s).

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1. Introduction

The problem of the inversion of a Laplace Transform consists in expressing a function f(t) in terms of its Laplace Transform F(s). The Weeks method [4, 6] is based on the following series representation, established first by Tricomi [5]:

$$f(t) = e^{\sigma t} \sum_{k=0}^{\infty} a_k e^{-bt/2} L_k(bt), \qquad (1.1)$$

where the coefficients a_k are the Taylor coefficients of

$$\Phi(z;\sigma,b) = \frac{b}{1-z} F\left(\frac{b}{1-z} + \sigma - b/2\right) = \sum_{k=0}^{\infty} a_k z^k, \quad |z| < R_{\phi}(\sigma,b), \quad (1.2)$$

 $\sigma > \sigma_0$, b > 0 are parameters, and $L_k(x)$ is the k-th Laguerre polynomial. As usual, σ_0 denotes the abscissa of convergence of the Laplace Transform F(s), which can be defined as the maximum of the real parts of the singularities of F(s).

In the sequel we will consider only the class A of the Laplace Transform functions F(s) which are regular at infinity and such that

$$F(\vec{s}) = \overline{F(s)},$$

$$F(s) = \mathbf{O}\left(\frac{1}{s^{\nu}}\right), \quad \nu \ge 1, \text{ as } s \to \infty.$$

When $F \in \mathbf{A}$, series (1.1) is absolutely and uniformly convergent.

In (1.1) there are two arbitrary parameters σ and b, that also characterize the particular Möbius mapping on which the method is based. The numerical performance of the method, i.e., its efficiency and accuracy, depends critically on the choice of these parameters [1, 3]. The choice of σ is related to the range of t to which (1.1) is applied. Series (1.1) converges slowly when $\sigma - \sigma_0$ is small (for $\sigma < \sigma_0$ there is no convergence) and faster when $\sigma - \sigma_0$ is larger. On the other hand, if series (1.1) is taken as basis of a numerical method, then the larger $\sigma - \sigma_0$, the smaller the range of t for which the numerical results are meaningful. Briefly, this is due to the factor $e^{\sigma t}$ in (1.1) which amplifies the approximation error arising in the computation of the coefficients a_k . In [1], it is shown that a sound choice of σ can be made if the range [0, T] of t is known: in this case, setting σ as $\sigma = \sigma_0 + 1/T \log(\varepsilon_T/\varepsilon_0)$, $\varepsilon_T > \varepsilon_0$, the relative accuracy of the numerical results degrades from ε_0 to ε_T .

The choice of b depends on σ and on analytical properties of F(s).

The aim of this paper is the determination of b_{opt} , the value of b to which corresponds to fastest convergence of series (1.1), once σ is fixed. In Sect. 2 we formally define b_{opt} and in Sect. 3 we show that b_{opt} depends only on σ and on the location of the singularities of F(s). The proof in Sect. 3 gives a geometric construction of b_{opt} for a given Laplace Transform F(s) and requires that the convex hull of the singularities of F(s) be finite. In Sect. 4 we report the results of numerical examples which illustrate the theory.

2. Definition of b_{opt}

We use a standard measure of the convergence rate of a series, i.e., among various series $\sum \alpha_k$, the one for which $\lim_{k \to \infty} \sup |\alpha_k|^{1/k}$ is least converges fastest.

It is easy to show that, for a fixed $\sigma > \sigma_0$, the rate of convergence of the series (1.1) depends only on $R_{\phi}(b)$ in (1.2): using a well-known property of the Laguerre polynomials, namely

$$\limsup_{k\to\infty} |L_k(x)|^{1/k} = 1,$$

and the Cauchy-Hadamard formula

$$|\limsup_{k\to\infty}|a_k|^{1/k}|^{-1}=R_{\boldsymbol{\sigma}}(b),$$

it follows that the fastest convergence of (1.1) is achieved when $R_{\phi}(b)$ is maximum. Thus we have Property 2.1. b_{opt} is the value of b which maximizes $R_{\phi}(b)$, i.e.,

$$R_{\boldsymbol{\phi}}(b_{\text{opt}}) = \max_{b>0} R_{\boldsymbol{\phi}}(b).$$
(2.1)

In order to get to a characterization of b_{opt} that permits the actual calculation of the optimal value of the parameter b, we need to further analyze the complex mapping in (1.2).

Definition 2.1. TW and its inverse TW^{-1} are the following Möbius transformations:

$$z = TW(s; \sigma, b) = \frac{s - \sigma - b/2}{s - \sigma + b/2}, \qquad s \in \mathbb{C},$$

$$s = TW^{-1}(z; \sigma, b) = \frac{b}{1-z} + \sigma - b/2, \quad z \in \mathbb{C}.$$

TW and TW^{-1} map the extended z-plane one-to-one onto the extended s-plane. (An extended plane contains ∞ as an element.)

Incidentally, the interest of the present authors in these mappings was derived also from a different context, namely the design of a numerical method for computing the abscissa of convergence σ_0 of a given Laplace transform [2].

The following lemmas provide necessary tools to prove the main theorem in Sect. 3.

In the sequel, we denote with $C[\rho]$ the circle which is the image in the s-plane (by TW^{-1}) of the circle $|z| = \rho$ in the z-plane.

Lemma 2.1. The circle $C[\rho]$ has center

$$\sigma + \frac{b}{2} \frac{1+\rho^2}{1-\rho^2}$$

and radius

$$\frac{\rho b}{|1-\rho^2|}$$

Lemma 2.2. If $F \in \mathbf{A}$, then $R_{\Phi}(\sigma, b)$ in (1.2) satisfies one of the following relations for all b > 0:

$$\sigma > \sigma_0 \Leftrightarrow R_{\Phi}(\sigma, b) > 1,$$

$$\sigma = \sigma_0 \Leftrightarrow R_{\Phi}(\sigma, b) = 1,$$

$$\sigma < \sigma_0 \Leftrightarrow R_{\Phi}(\sigma, b) < 1.$$

Proof. $TW(s; \sigma, b)$ maps the half plane $\operatorname{Re}(s) \ge \sigma$ into the circle $|z| \le 1$. If $\sigma = \sigma_0$, the relation follows from the previous property and the fact that $\Phi(z)$ is regular in z=1. Otherwise let us consider $z=TW(s; \sigma, b)$ for s such that $\operatorname{Re}(s) \ge \sigma_0$. If $\sigma > \sigma_0$, two possibilities can arise: $\sigma - b/2 \le \sigma_0 < \sigma$ or $\sigma_0 < \sigma - b/2$. The half plane $\operatorname{Re}(s) > \sigma_0$ is mapped, in the first case, in $|z-\delta| < r$, where $\delta < 0$, $r = |1-\delta|$, and, in the second case, in $|z-\delta| > r$, where $\delta > 1$, $r = |\delta - 1|$; in both the cases,

from the regularity of $\Phi(z)$ in z=1, we have $R_{\Phi}(\sigma, b) > 1$. Conversely, if $R_{\Phi}(\sigma, b) > 1$, consider the image (by TW^{-1}) of $|z| \le R_{\Phi}$ in the s-plane. By Lemma 2.1 it follows that $\sigma > \sigma_0$.

If $\sigma < \sigma_0$ then $\operatorname{Re}(s) > \sigma_0$ is mapped in $|z-\delta| < r$, where $0 < \delta < 1$, $r = |1-\delta|$, which implies $R_{\phi}(\sigma, b) < 1$. Conversely, if $R_{\phi}(\sigma, b) < 1$, then again from Lemma 2.1 there follows $\sigma < \sigma_0$. \Box

Let us consider the circle $C[R_{\Phi}(b)]$ and let r(b), c(b) be its radius and its center, respectively; then by Lemmas 2.1, 2.2, since $\sigma < \sigma_0$, it follows that $c(b) + r(b) < \sigma$, $\forall b > 0$.

Moreover, since the circle $|z| \ge R_{\phi}(b)$ is mapped by TW^{-1} into the region outside the circle $C[R_{\phi}(b)]$, all the singularities of F(s) belong to $C[R_{\phi}(b)]$.

Lemma 2.3. The tangent segment from σ to $C[R_{\phi}(b)]$ has length equal to b/2.

The proof is almost trivial and consists in applying Pythagoras's theorem to the triangle which has the tangent segment from σ and the radius of $C[R_{\phi}(b)]$ as legs.

3. Geometric Characterization of b_{opt}

The main result of this paper is the following theorem, in which we show that b_{opt} is the value of b that minimizes the angle between the tangent segment from σ to $C[R_{\varphi}(b)]$ and the real axis.

Theorem 3.1. Let $2\beta(b)$ be the angle subtended by $C[R_{\phi}(b)]$ at σ ; then

$$\beta(b_{opt}) = \min_{b} \beta(b).$$

Proof. Since $0 < \beta(b) < \pi/2$, finding $\min_{b} \beta(b)$ is equivalent to finding $\min_{b} \tan \beta(b)$, where

$$\tan \beta(b) = \frac{2 R_{\Phi}(b)}{[R_{\Phi}(b)]^2 - 1}.$$

If we choose $b \neq b_{opt}$, then $R_{\phi}(b) \leq R_{\phi}(b_{opt})$ and, after elementary calculations, we have

$$\tan \beta(b) = \frac{2R_{\phi}(b)}{[R_{\phi}(b)]^2 - 1} \ge \frac{2R_{\phi}(b_{\text{opt}})}{[R_{\phi}(b_{\text{opt}})]^2 - 1} = \tan \beta(b_{\text{opt}})$$

and the proof is completed. \Box

Moreover, there exists just one value of b that maximizes R_{ϕ} , as stated by the following corollary.

Corollary 3.1. The value of b_{opt} defined in (2.1) is unique.

Proof. From Theorem 3.1, b_{opt} characterizes $C[R_{\Phi}(b_{opt})]$ as the circle, with center on the real axis, including all the singularities of F(s), and with minimum angle subtended by its tangent at σ . Since the circle having these properties is uniquely determined, so is the length of the tangent segment at σ , i.e., b_{opt} .

Thus we have shown that, once a Laplace Transform F(s) and $\sigma < \sigma_0$ are given, the circle $C[R_{\sigma}(b_{opt})]$ is the circle, with center on the real axis and including all the singularities of F(s), which subtends the smallest angle at σ ; by Lemma 2.3 the numerical value of $b_{opt}/2$ is simply the length of the tangent segment from σ to $C[R_{\sigma}(b_{opt})]$.

The following additional properties allow the construction of $C[R_{\phi}(b_{opt})]$ once that σ and the singularities $s_i, j = 1, ..., m$ of F(s) are given:

 $C[R_{\phi}(b_{opt})]$ passes through only one singular points pair s_k , \bar{s}_k if and only if the tangents to it at s_k and \bar{s}_k pass through σ .

 $C[R_{\phi}(b_{opt})]$ passes through two pairs $(s_k, \bar{s}_k), (s_j, \bar{s}_j), k \neq j, 1 \leq k, j \leq m$ and the length ℓ of the tangent from σ to it $(\ell = b_{opt}/2)$ is such that

$$|\sigma - s_k| \leq \ell \leq |\sigma - s_j|.$$

This geometric construction of b_{opt} is quite straightforward and can be easily carried out in practical applications to assign in Weeks's method, or some of its algorithmic versions, the best value of the parameter *b*. In some cases a good choice of the value of *b* is needed to get meaningful results.

This is especially true if Weeks's method is used for the real inversion problem, i.e., F(s) is known or can be computed only on the real axis. In this case the need for fast convergence of (1.1) may be critical, because the roundoff error affects the computation of the coefficients a_k , and only the first few of them can be computed in a reliable way.

In most of the practical cases, an explicit form of F(s) in the whole complex plane is rarely available. We emphasize that, if only the location of some of the singularities of F(s) is known, our characterization of b_{opt} allows the calculation of an approximate value and moreover, it can be seen that such an approximation is better if the rightmost singularities of maximum imaginary part are known.

4. Numerical Results

In this section we report some results of the numerical experiments that we have carried out. Let $\tilde{f}_m(t)$ be an approximation of f(t) in (1.1) given by

$$\tilde{f}_m(t) = e^{\sigma t} \sum_{k=0}^m a_k e^{-bt/2} L_k(bt)$$
(4.1)

and let $E_m(f, t)$ be the corresponding relative error

$$E_m(f,t) = \left| \frac{f_m(t) - f(t)}{f(t)} \right|.$$



Fig. 1. Number of terms N in (4.1) as function of b, for various required accuracies. Test function is (4.3), $\sigma = 2$, t = 2, b_{opt} is 5



Fig. 2. Number of terms M in (4.1) as function of b, for various required accuracies. Test function is (4.3), $\sigma = 2$, t = 8, b_{opt} is 5

For a given Laplace Transform function F(s) the aim of the experiment is to find N such that

$$N = \min\{m \mid E_m(f, t) < \varepsilon\},\tag{4.2}$$

once that σ , b, t, ε are given.

In the example we use the function

$$F(s) = \frac{1}{s} + \frac{1}{s+2\alpha} + \frac{1}{(s+\alpha)^2 + \alpha^2},$$
(4.3)

which has four simple poles in 0, -2α , $-\alpha + i\alpha$, $-\alpha - i\alpha$. We set $\sigma = 2$, $\alpha = 0.5625$ and we obtain, using Theorem 3.1, $b_{opt} = 5$. The coefficients a_k in (4.1) are computed exactly by analytic differentiation of the function $\Phi(z; \sigma, b)$ in (1.2).

In Figs. 1 and 2 the behavior of N as a function of b is shown for t=2 and t=8, respectively, and for three values of the required relative accuracy ε .



Fig. 3. Number of terms N in (4.1) as function of b, for various t. Test function is (4.3), $\sigma = 2$, $\varepsilon = 10^{-6}$, b_{opt} is 5

In Fig. 3, ε is fixed ($\varepsilon = 10^{-6}$) and again N, as a function of b, is plotted for several values of t.

Floating-point arithmetic with machine precision $\varepsilon_M = 0.17 \times 10^{-7}$ has been used.

In some cases this machine precision causes a numerical cancellation that prevents us from achieving the required accuracy: this is shown by a vertical asymptote in the graph.

The numerical results obtained confirm the theory. They also show that N(b) increases slowly for $b > b_{opt}$ while it grows faster for $b < b_{opt}$; such a behavior becomes even more evident when t is large.

These conclusions suggest that, if in a practical application of Weeks's method the exact value of b_{opt} is not known, an overestimated approximation of b_{opt} will likely provide acceptable speed of convergence.

In the example reported here, the coefficients a_k in (4.1) have been computed exactly, since we dealt with the rate of convergence of (1.1), i.e., we focused on the behavior of the truncation error of the approximation (4.1) in terms of b. Numerical implementations of Weeks's method primarily concern about computational schemes for approximating the coefficients a_k . In [4, 6], the a_k 's are computed using numerical integration over a complex contour and in [4] it has been shown that the faster the series (1.1) converges the smaller the discretization error of the two algorithms. Experimental results, obtained in the test process of the software in [1], show that the behavior of the global approximation error is similar to that of N(b) in the previous example.

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